DIAMOND NANOWIRES GROWN INSIDE CARBON NANOTUBES UPON CHEMICAL VAPOR DEPOSITION: THERMODYNAMIC AND KINETIC APPROACH

C. X. Wang, P. Liu, H. Cui, G. W. Yang

State key laboratory of optoelectronic materials and technologies, School of Physics Science & Engineering, Zhongshan University, Guangzhou 510275, P. R. China

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Abstract

One-dimensional nanostructures such as wires, rods, belts, and tubes have become the focus of intensive research owing to their unique applications in mesoscopis physics and fabrication of nanoscale devices. Due to several unique properties including extreme high hardness, very high thermal conductivity, large band gap, and chemical inertness, etc., diamonds are expected to be an important semiconductor material for high-temperature and high-power microelectronics device, and UV-light emitting optoelectronics. Very recently, one-dimensional nanostructures of diamond have received increasing interesting in theoretical. For example, due to stronger than fullerene nanotubes, diamond nanorods are expected to be an important and viable target structure for synthesis. Barnar's studies indicate that the energy band gap of diamond nanowires (DNWs) is significantly reduced, due to the contributions from occupied and unoccupied surface states. However, up to date, any successful syntheses of diamond nanowires have not been found in the literature yet, to our best knowledge. On the other hand, carbon nanotubes (CNTs) have many potential applications as molecular sieves, membranes, and "nanopipes" for precise delivery of gases or liquid. Furthermore, some studies focused their attentions on transport, adsorbed, and condensed phases of gases inside CNTs. Especially, the transport rates of CH_4 and H_2 gases in CNTs were suggested to be exceptionally high. Interestingly, CH_4 and H_2 gases are just two typical reactive gases that are employed to deposit diamond films upon chemical vapor deposition (CVD). These studies mentioned above naturally imply that CNTs could be expected to be a possible path to fabricate DNWs by CVD. In this study, we propose a nano-scaled thermodynamic nucleation and growth kinetic approach in theoretical, with respect to the effect of nanosize-induced surface tension, for the formation of DNWs inside CNTs upon CVD. Thermodynamic analyses show that the diamond nucleation inside a CNT would be preferable to that on the flat surface of silicon substrate due to the effect of surface tension induced by the nanosize curvature of CNTs. Meanwhile, the capillary effect of the nanosize curvature of diamond nuclei could drive the metastable phase region of diamond nucleation into a new stable phase region in the carbon thermodynamic equilibrium phase diagram. Kinetic analyses indicate that the growing rate of DNWs would go to much high once nuclei formed inside CNTs, due to the same nanosize-induced effect. Eventually, we predict that CNTs could be an effective route to grow DNWs by CVD.